# 3-Pyridineacetonitrile

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|---|---|
| **Other names:** | 3-Cyanomethylpyridine |
| | 3-Pyridylacetonitrile |
| **Inchi:** | InChI=1S/C7H6N2/c8-4-3-7-2-1-5-9-6-7/h1-2,5-6H,3H2 |
| **InchiKey:** | OIPHWUPMXHQWLR-UHFFFAOYSA-N |
| **Formula:** | C7H6N2 |
| **SMILES:** | N#CCc1cccnc1 |
| **Mol. weight [g/mol]:** | 118.14 |
| **CAS:** | 6443-85-2 |

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| log10ws | -1.91 | | Crippen Method |
| logp | 1.148 | | Crippen Method |
| mcvol | 97.090 | ml/mol | McGowan Method |

## Pressure Dependent Properties

| Property code | Value | Unit | Pressure [kPa] | Source |
|---|---|---|---|---|
| tbrp | 378.20 | K | 0.10 | NIST Webbook |

## Sources

| | |
|---|---|
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=C6443852&Units=SI |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| **Crippen Method:** | https://www.chemeo.com/doc/models/crippen_log10ws |
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |

# Legend

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|---|---|
| **log10ws:** | Log10 of Water solubility in mol/l |
| **logp:** | Octanol/Water partition coefficient |
| **mcvol:** | McGowan's characteristic volume |
| **tbrp:** | Boiling point at reduced pressure |